

S. A.
Sect. A

Cryptography

548.733
2209. Finding the coordinates of the atoms in the unit cell of a crystal by means of the P^* -series. A. I. Karalennikov. *Zh. Eksp. Teor. Fiz.*, 21, 717-30 (Mar. 6, 1951) in Russian.

It is shown that the endpoints of any interatomic vector of the P^* -series is a centre of inversion which connects two groups of points each of which represents the structure of the crystal. The possibility of uniquely deriving a structure from its representation as a 3-dimensional P^* -series has been shown by Shorger (Abstr. 3517 (1950)), and the practical scheme for doing this which is developed here follows observations by Bragg and Zhdanov (Abstr. 9117 (1938)). Three-dimensional P^* -series are necessary, and a calculation is added showing that the practical solution of a structure (all the atoms of which are approximately the same weight) is likely to be possible.

A. L. MACRAY

CA

2

X-ray structure investigation of 1,3-dichloronaphthalene.
 A. I. Kholodnyukh and N. S. Kabalkina (Inst. Org. Chem.,
 Moscow). *Dokl. Akad. Nauk SSSR*, 23, 71-81 (1961).—The di-
 mensions of the unit cell of 1,3-dichloronaphthalene are:
 $a = 15.00 \pm 0.1$; $b = 4.10 \pm 0.02$; $c = 14.3 \pm 0.3$ Å;
 $\beta = 92^\circ 28' \pm 8'$; 4 mol. per unit cell; space group C_2
 ($A2/c$). Two at. coordinates are first detd. from the re-
 flection intensities, then the orientation of the mol. is calcd.
 and the third coordinates are deduced from it. The struc-
 ture is verified by the good agreement between the calcd.
 and exper. structure amplitudes, *F*, e.g., for $hkl = 201, 400$,
 $011, 201, 012, 013$, $F_{\text{calcd.}} = 40, -42, 50, -42, 18$,
 9 , and $F_{\text{exper.}} = 41, 52, 64, 43, 16, 8$. The bond distances are
 (in Å.): C₁-C₂, 1.46; C₂-C₃, 1.23; C₃-C₄, 1.23; C₄-C₅, 1.37;
 C₁-Cl, 1.76; C₅-Cl, 1.20. The error is estd. at ± 0.08 Å.
 These results agree well with the bond distances found for
 naphthalene (Abraham, *et al.*, *C.A.*, 44, 15725). The Cl
 atom probably displaces C₅ by approx. 0.02 Å, which is
 toward the exper. error. Michel Boudart

1967

CA

Possibility of determining the center of symmetry of a crystal by x-ray structure analysis. A. I. Kitaigorodskii. *Zhur. Fiz. Khim.* 23, 157-8 (1941).—This possibility, as shown by Wilson (*Acta Cryst.* 2, 214 (1949)) rests on the fact that $(F_0)/F_0$ is equal to $1/4$ (0.25) when there is no symmetry center and to $1/2$ (0.5) when there is one. These are, however, limiting cases and it is conceivable that the ratio may take any value between 0.25 and 0.5. The method succeeds in proving the absence of the symmetry center but fails in proving its presence. In the work of Howells, et al. (*C.A.* 44, 5786a) crystals known to have a symmetry center give ratios of the order of 0.64-0.70, whereas known nonsymmetric structures give $(F_0)/F_0 = 0.76$, whereas known symmetric structures give $(F_0)/F_0 = 0.76$. The method fails in nontrivial cases; e.g. the quoted authors assign $(CaF_2)_2$ to the space group $P2_1/a$. This is incorrect; as in many analogous cases, the packing of org. units in this group is difficult, the 2 axis (thus the inversion center) is lost and the group P_2 is formed with 4 units (2 nonequiv.) per unit cell. The units in such a crystal are very densely packed and their arrangement differs only little from a structure possessing an inversion center (cf. *C.A.* 43, 538a).
Michel Boudart

CA

2

Crystal structure of bisoform. A. A. Khatayevich, E. I. Khosyanova, and Yu. I. Strumkin (Izv. Vys. Chem., Acad. Sci. USSR, Moscow: *Uch. Zap. Kaz. S.S.S.R.* 78, 1161-6/1971). The space group C_{2h}^2 is chosen unambiguously from 2 possible groups on the basis of the symmetry of the node. The coordinate z_1 of the I atom can be chosen arbitrarily. The other 2 coordinates are fixed from the projection of the P^2 atom on the ab face, the corrected values are $x_1 = 0.354 \pm 0.002$, $y_1 = 0.001 \pm 0.002$. Taking $x_1 = 0.320$, one finds for the C atom $x_2 = 0.310 \pm 0.001$, in very good agreement from the P^2 and P^1 series. The C(II) atom is tetrahedral, with the valence angles H-C-I and I-C-I = $109^\circ 24' \pm 0^\circ 20'$, bond distance C-I = 2.18 ± 0.002 Å. The I-I distance within the node is 3.50 Å, the distance between I atoms of nodes along the b axis in the ab layer is 3.06 Å. Each I atom of one node touches 2 I atoms of 2 neighboring nodes. Thus, in the ab layer, the node coordination is 12. The distance between I atoms of nodes along the axis b in the ab layer is 4.31 Å. The layers are staggered along the axis z_1 , the I-I distance along that axis, i.e. from one layer to another, is 4.11 and 4.41 Å. The C atom is at a distance of 3.95 Å from the nearest I atom of the neighboring node, and the H at a distance of 3.14 Å (if the C-H distance is taken = 1.09 Å). The only contacts between layers are H-I. Each H atom touches 3 I atoms of the node of the following layer, and each I atom takes part in one contact I-H. The node coordination is 12. This packing is evidently the closest possible in this case.

N. Tsim

Kitaigorodskii, A. I., and Merzhtsev, V. A.: Atomi i molekuly (Atoms and Molecules). Moscow: State Pub House Cultural and Ed. Lit. 1952. 76 pp.

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PHASE I Treasure Island Bibliographic Report

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BOOK

APPROVED FOR RELEASE: 09/17/2001

CIA-RDP86-00513R000722920003-6

Author: KITAIGORODSKII, A. I.

Full Title: X-RAY STRUCTURAL ANALYSIS OF MICROCRYSTALLINE AND AMORPHOUS SUBSTANCES.

Transliterated Title: Rentgenostrukturnyi analiz melkokristallicheskih i amorfnykh tel.

Publishing Data:

Originating Agency: None.

Publishing House: State Publishing House of Technical-Theoretical Literature.

Date: 1952.

No. pp.: 588

No. of copies: 6,000

Editorial Staff

Editor: None.

Tech. Editor: None.

Editor-in-Chief: None.

Appraiser: None.

Text Data

Coverage: The book which is a continuation of another work by the same author entitled X-Ray Structural Analysis, 1950, describes the application of X-Ray structural analysis to the study of amorphous and microcrystalline substances, irregular crystals, and other substances. Pt.I: X-Ray diffraction by amorphous, quasi-crystalline, and polycrystalline substances. Pt.II: Data on X-Ray structural analysis (Hydrocarbons and their derivatives, proteins, cellulose, animal tissues, fats and soap, coal, inorganic compounds, metals, and polycrystalline substances). Tables of distances between planes and relative intensities of lines in X-Ray graphs for 1299 polycrystalline substances pp. 417-578). Subject index.

Purpose: A textbook for engineers and scientific personnel; also, for students of advanced courses in technical institutions of higher learning.

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Card 2/2

Call No.: QD945.K55

Full Title: X-RAY STRUCTURAL ANALYSIS OF MICROCRYSTALLINE AND AMORPHOUS SUBSTANCES

Facilities: None.

No. of Russian References: References appear only in footnotes.

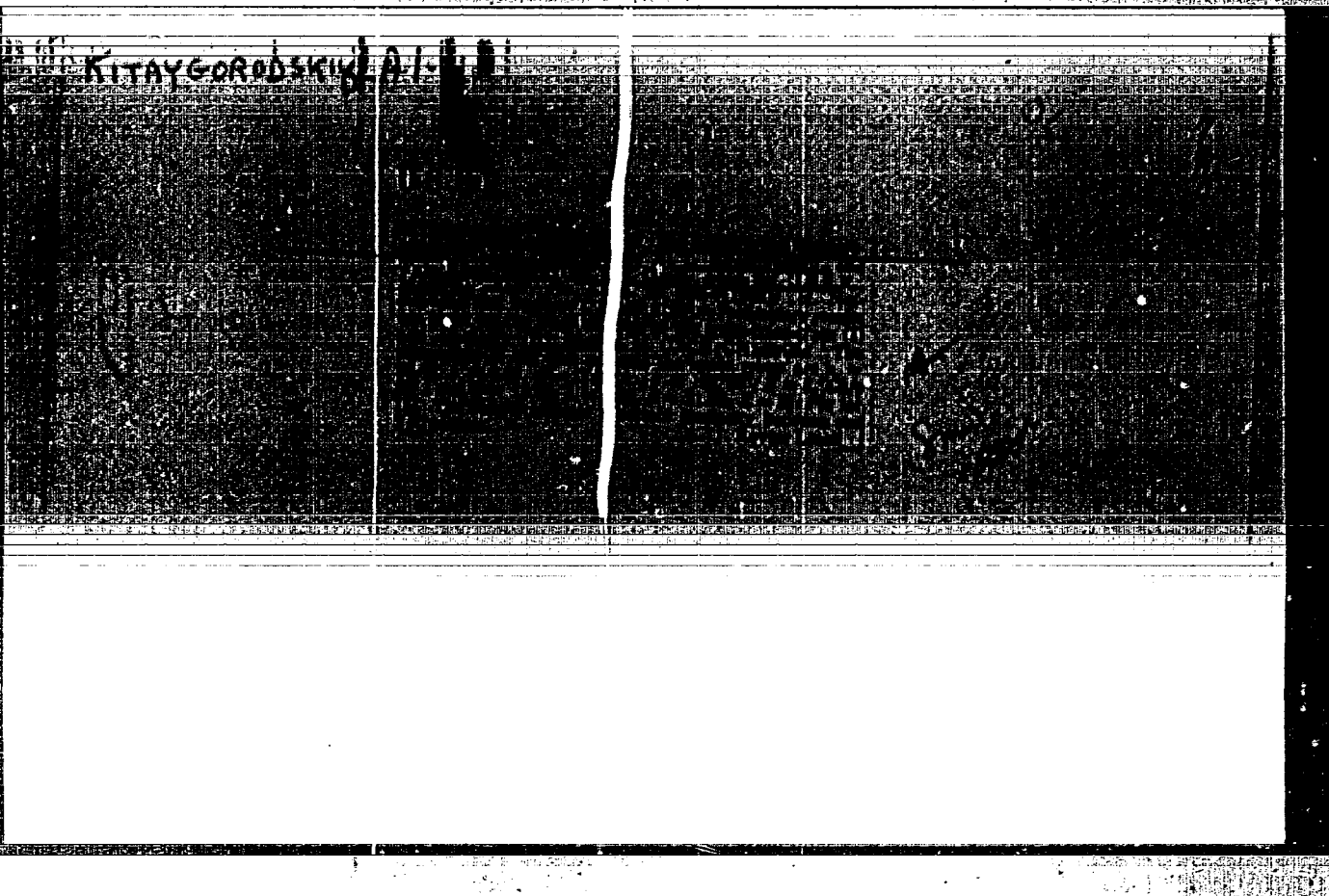
Available: Library of Congress.

KLIMENKOV, V.S.; KAROIN, V.A.; KITAYGORODSKIY, A.I.

Density of packing of highly polymeric compounds. Khim. i Fis.
Khim. Vysokomolekul. Soedineniy, Doklady 7-oy Konf. Vysokomolekul.
Soedineniyam '52, 231-41. (MLRA 5:7)
(CA 47 no.15:7817 '53)

"APPROVED FOR RELEASE: 09/17/2001

CIA-RDP86-00513R000722920003-6



APPROVED FOR RELEASE: 09/17/2001

CIA-RDP86-00513R000722920003-6"

KITAYGOLOVSKIY, A.I. Prof.

Science

Undertaking of great importance; (On the popular science library of the State Technical Publishing House). Priroda 41, No. 6, 1952.

Monthly List of Russian Acquisitions, Library of Congress, September 1952. UNCLASSIFIED

KITAYGORODSKIY, A.L. PROF.

Symmetry

Something new about symmetry. Perioda 41 no. 7, 1952

Inst. of Organic Chemistry, AS USSR

Monthly List of Russian Accessions, Library of Congress, November 1952. UNCLASSIFIED

KITAYGORODSKIY, A. I.

USSR/Physics - Solid State Physics

Jan 52

"Progress in X-Ray Structural Analysis of Crystals,"
A. I. Kitaygorodskiy

"Uspekhi Fiz Nauk" Vol XLVI, No 1, pp 23-70

Brief exposure of theoretical computation of diffraction by crystal lattice with reference to book by himself (cf. "X-Ray Structural Analysis" 1950). Defines structure of crystals by interatomic vectors, determines phases of structural amplitudes, series of electron densities and discusses possibilities of X-ray analysis.

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KITAYGORODSKIY, A. I.

USSR/Physics - Crystals

Jul 52

"New Method of Determination of Complex Structures of Crystals," A. I. Kitaygorodskiy

"Uspekhi Fiz Nauk" Vol XLVII, No 3, pp 487-489

Essence of subject method is as follows: from the intensities of the X-ray reflections one calculates the structural amplitudes F_H by the usual familiar procedures and reduces the values of F to an abs scale also by familiar methods; then by usual methods of averaging the mean atomic factors are found, after which one possesses knowledge of the abs magnitudes of unit structural amplitudes U_H for each reflection; that is, amplitudes such that are equal to unity if all atoms scatter in one phase.

225T102

KHOTSYANOVA, T.L.; KITAYGORODSKIY, A.I.; STRUCHKOV, Yu.T.

Crystal structure of tetraiodoethylene, C_2I_4 . Doklady Akad. Nauk
S.S.S.R. 85, 785-8 '52. (MLRA 5:8)
(CA 47 no.16:7854 '53)
(PA 56 no. 671: 7096 '53)

1. KITAYGORODSKIY, A. I., Prof.

2. USSR (600)

4. Molecular Theory

7. Atomic structure of matter. Viz v shkole No 1 1953.

9. Monthly List of Russian Accessions, Library of Congress, April 1953, Uncl.

KITAY GERODSKY, A.I.
Kitaygerodskiy, A. I.

USSR.

541 735

7875. The statistical method of determining the signs of the structure amplitudes. A. I. Kitaygerodskiy, *Letter in Zh. eksp. teor. Fiz.*, 24, No. 6, 747-8 (1953) in Russian.

The relationship (sign F_{hkl}) (sign $F_{h'k'l'}$) = (sign $F_{h+k, l+l'}$) is deduced and an expression for the limits of its validity is derived. If $x = F_{hkl} F_{h'k'l'}$, $F_{h+k, l+l'}$ and $y = 2(\sigma^2/\Sigma^2)$, then W , the probability that x is positive, is given by $1/W = 1 + \exp(-xy/\Sigma^2)$. The probability that the sign relationship is true is greater when σ^2/Σ^2 is small, the latter term being a minimum when there are heavy atoms in the cell. The signs of strong reflections are almost certain; i.e. when l is large. In the least favourable case of identical atoms the lowest probability for 25 atoms is 85% and for 100 atoms 70%.

AB
EW

KITAYGORODSKIY, A. I.

7

Low-temperature study of the structure of aromatic compounds. I. Anisotropic thermal expansion of α -naphthalene. V. M. Koshin and A. I. Kitaygorodskiy (USSR, Leningrad Univ., USSR, Leningrad, 211700). Zh. Fiz. Khim. 57: 101-110 (1983). X-ray measurements were made on a single crystal. The dimensions of the unit cell at 20° are $a = 4.214 \pm 0.005$, $b = 5.720 \pm 0.001$, $c = 8.661 \pm 0.005$ Å, $\beta = 122.55^\circ \pm 10'$; at -145° these are 8.108, 5.938, 8.616 Å, 126.00° . The coeffs. of expansion along the main and minor axes of the mol. are 22.8 and 60.5, normal to the plane of the mol. 163.7 (10^{-6}). The an. values for the principal coeffs. of expansion are $\alpha_{11} = 212.8 \pm 4.0$, $\alpha_{22} = 40.3 \pm 0.4$, $\alpha_{33} = 6.15$ or 5.1 ± 0.1 (10^{-6}). (If the value of 6.15 is given in the summary, the value 5.1 in the body of the article). α_{33} coincides with axis b , α_{11} forms an angle of $44^\circ 10'$ with axis a . R. F. Meyer.

PA 56 no 672-8798 (3)

KITAY - KIRILLOV, D. I.

Chemical Abstracts
Vol. 48 No. 5
Mar. 10, 1954
General and Physical Chemistry

Crystal structure of iodolene. T. L. Khramov, A. I. Kitalovskii, and V. P. Gerasimov (Inst. of Org. Chem., Acad. Sci. U.S.S.R., Moscow). *Zh. Fiz. Khim.* 27, 647-64 (1953); cf. C.A. 47, 7854a. — The crystal structure of CHI₃ was detd. by x-ray diffraction. The valence angle I-C-I is $109 \pm 8^\circ$. The bond length C-I is 2.18 ± 0.06 Å., 0.06 Å. more than the value found by Bastiansen by electron diffraction. The distance between I atoms within the mol. is 3.66 Å. The spatial arrangement of the mol. is described and discussed. J. W. Lowery, Jr.

Handwritten initials and date: "K-22-54"

KITAY GORODSKIY, A.I.

5

U S S R .

4018. The crystal structure of iodine. A. I. KITAYGORODSKIY, I. L. KHOTIMSKAYA AND YU. I. KITAYGORODSKIY. Zh. fiz. khim., 27, no. 6, 780-1 (1953)

In Russian.
The crystal structure of iodine has been re-determined with results substantially in agreement with earlier work. Atoms lie in (*f*) positions in the space group *Cmcb* with (*z, z*) parameters (0.149, 0.113). The 121 observed reflections were corrected for absorption and used to give a Patterson section at *y* = 0. The molecular I-I distance was found to be 2.68 ± 0.01 Å, interlayer distances to be 3.36 and 4.04, and I-I distances between layers 4.35 and 4.38 Å. The form of the molecule is shown in a diagram.

A. I. KITAYGORODSKIY

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PM

KITAYGORODSKIY, A.I.

Chemical Abstr.
Vol. 48 No. 6
Mar. 25, 1954
General and Physical Chemistry

Packing densities of high polymers compounds.
Mikhailov, V.A. *Kolloid. Zh.* 16, No. 1, 1954, 1-4.
The packing densities of high polymers compounds, as well as for the corresponding polymers, in order to find the mol. contraction of 27rd the monomers, is calculated for each. The symbols λ_1 and the packing coefficients λ_2 and λ_3 for each. The symbols are defined by the expressions $\lambda_1 = V_p - V_m$, $\lambda_2 = V_p - V_m$ and $\lambda_3 = V_p - V_m$, where V is the sum of the radii of the atoms of the monomers, V_p is the sum of the radii of the atoms of the polymer, V_m is the sum of the radii of the atoms of the monomers. The degree of contraction is greater with flexible mol. chains than with rigid ones.

KITAYGORODSKIY, A I

USSR :

Crystal structure of tetralodoethylene. T. I. Kiselevskaya, A. I. Kitaygorodskii, and Yu. T. Struchkov (Inst. Org. Chem., Acad. Sci. U.S.S.R., Moscow). *Zhur. Fiz. Khim.* 37, 1320-13 (1963); cf. C.A. 47, 7854d, 49, 2145q. -- The cryst. structure of $C_{10}H_8$ was deter. by x-ray diffraction. The parameters of the monoclinic unit cell (a , b , c , and β) are 15.10 ± 0.05 , 4.45 ± 0.02 , 13.00 ± 0.04 Å, and $109 \pm 1^\circ$, resp. The unit cell has 4 mols.; the ρ_{calc} is 1.08. The space group is $C_{2h}^2/P2_1/c$. Within the mol. the distances C to C, C to I, and I to I, calcd. by means of a 3-dimensional electron-d. plot, are 1.34, 2.15, and 3.64 Å, resp., and the angles I-C-I and I-C-C are 115.7° and 123.15° , resp. The internod. dist. of I and C are 2.00 and 1.80 Å, resp. Coordinates of the atoms in the lattice are tabulated; the arrangement of the mols. in the crystal is depicted with illustrations. J. W. Lowrey, Jr.

KITAYGORODSKIY, A.I.

USSR.

The method of stereographic analysis used in the study of the crystal structure of tetraiodophthalic A. I. Kitagorodskii, T. L. Khochimskaya, and Yu. P. Gerasimov, *Dokl. Akad. Nauk SSSR*, Moscow, 1960, *Russ. J. Chem.*, 1961, 35, 87; English transl., *J. Am. Chem. Soc.*, 83, 1961, 1933; *J. Appl. Cryst.*, 1961, 4, 169. A mathematical discussion. An objective method is proposed for the conversion of the results of relative measurements of F_{obs} and F_{calc} to absolute units and the calculation of the mean factors. The validity of the n -factor formula $f = \frac{n}{n+1}$, where n and a are constants, and $s = 4 \pi m / \lambda$ is shown. Methods are given for determining the coordinates of atoms along one axis if the remaining coordinates are known, and for determining the coordinates of atoms in two- and three-dimensional series. Formulas for the probable error of determination of electron density are given and applied to x-ray diffraction data. The determination of light atoms in the presence of heavy ones is discussed. J. W. L. H.

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F A L S E H O O D

KITAYGOLOVSKIY, A. I.

Chemical Abstracts
May 25, 1954
General and Physical
Chemistry

Crystal structure of products of addition of coumarin and mercuric chloride and bromide. Yu. T. Strychkov, A. I. Kitaygolovskiy, and T. I. Kholodavich. *Doklady Akad. Nauk S.S.S.R.* 93, 675 (1953). X-ray analysis of coumarin-HgCl₂ (I) and coumarin-HgBr₂ (II) addn. compds. was made. Both are hemispherical with space group P2₁/a on monoclinic syngony. There are 4 mols. per unit cell, whose dimensions are: I a 23.63 Å, b 11.27, c 4.03, β 97°40', V 1004 cu. Å; II 24.01, 11.31, 4.10, 97°30', 1108 cu. Å. The products are not added at the double bond of coumarin. The shortest Hg-Cl distance in a crystal of I is 3.3 Å, and the products I and II are mol. compds. like RC(O)₂HgX, Cl atoms are at equal distance (2.33 Å) from Hg, with 171° angle. The Hg-O₂ distance is 2.38 Å. The mols. are closely packed on the c axis, forming a twinned ribbon of octahedral ClHgO units. The following interat. distances are abnormal: C-O (C in the 2 position) is slightly shortened; C=O is lengthened. Probable displacements are shown on diagrams. In II the shortening of Hg-O is less (2.73 Å). G. M. K.

KITAYGORODSKIY, Aleksandr Isaakovich, doktor fiziko-matematicheskikh nauk,
professor; LASHKOVICH, V.A., redaktor; KIPNIN, S.Ye., redaktor;
DMITRIYEVA, R.V., tekhnicheskij redaktor.

[Physical principles of atomic energy] Fizicheskie osnovy iadernoi
energetiki. Moskva, Izd-vo "Znanie," 1954. 38 p. (Vsesoiusnoe ob-
shchestvo po rasprostraneniю politicheskikh i nauchnykh snanii,
Ser. 3, no.57) (MLRA 7:12)
(Atomic energy)

KITAYGORODSKIY, A.I.; VOL'KENSHTEYN, M.V., redaktor; BELOVA, V.I.,
redaktor; ASTAF'YEVA, O.A., tekhnicheskiy redaktor.

[Order and confusion in the world of atoms] Poriadok i bes-
poriadok v mire atomov. Moskva, Izd-vo Akad. nauk SSSR,
1954. 69 p. (MLRA 7:12)
(Atoms) (Crystallography)

KITAYGORODSKIY, Aleksandr Isaakovich; MEZENTSEV, Vladimir Andreyevich;
KRIVOSHENYA, A.S., redaktor; ATAMASHKO, V.P., tekhnicheskij redaktor.

[Atoms and molecules] Atom i molekula. Pereklad z rosijs'koho
vydannya. Kyiv, Derzh.naukovo-pedahoh.vyd-vo "Radiana's'ka shkola,"
1954. 83 p. (Microfilm) (NLRA 8:2)
(Atomic theory)

KITAYGORODSKIY, A.I.

"Theory of the Determination of Indicators of Structural Amplitudes." by
A.I. Kitaygorodskiy, pp. 27-41

SO: Works of the Inst. of Crystallography, Issue #10, (Reports submitted
at the 3rd International Congress of Crystallography; published by
the Acad Sci USSR, Moscow, 1954)

KITAYGORODSKIY, A. (Prof.) (Dr. Physicomathematical Sci.)

"Atomic Energy," a 3-page article discusses in general the chemistry of the atomic nucleus, including nuclear reaction of uranium isotopes 235, in some detail, and 238 briefly; a nuclear reaction with a graphite moderator in detail, and with heavy water briefly.

Kryl'ya Rodiny, No 5, pp 18,19,20, May 1954

~~KITARYGORODSKIY, A.I.~~ professor, doktor fiziko-matematicheskikh nauk
(Moscow)

Nuclear power engineering. Fiz.v shkole 14 no.6:3-14 M-D '54.
(Nuclear reactors) (MLRA 7:12)

KITAYGORODSKIY, A. I.

USSR/ Physics - Analyses methods

Card 1/1 Pub. 13 - 9/62

Authors : Kitaygorodskiy, A. I.

Title : Elastic constants and the configuration of a molecule

Periodical : Izv. AN SSSR. Ser. fiz. 18/6, 664-665, Nov-Dec 1954

Abstract : A brief survey is given showing how the spectral and x-ray structural analysis methods make it possible to determine the configuration of molecules. X-ray structural analysis determines the structure and configuration of the molecule and the elasticity constants of valent angles are established spectroscopically. If it is assumed that the intermolecular forces vary linearly with the deformation of the atoms then each atom can be individually characterized by the compressibility coefficient.

Institution : Acad. of Sc., USSR, Inst. of Elementorganic Compounds

Submitted :

KITAI GORODSKI A.I.

Kitalgorodskij, A. I. The theory of the statistical method of structure analysis. Dokl. Akad. Nauk SSSR (N.S.) 94, 225-228 (1954). (Russian) I - F/W

KITAYGORODSKIY, Aleksandr Issakovich

[Crystals] Kristally. 1zd.3. Moskva, Gos.izd-vo tekhn.-teoret.
lit-ry, 1955. 62 p. (Nauchno-populiarnaya biblioteka, no.19)
(MIRA 13:3)

(Crystallography)

KITAYGORODSKIY, A.I., professor; KADER, Ya.M., redaktor; MIKHAYLOV, V.A.,
kandidat fiziko-matematicheskikh nauk, inzhener-podpolkovnik;
SOROKIN, V.V., tekhnicheskii redaktor.

[Structure of matter and its energy] Stroenie veshchestva i ego
energii. Moskva, Voen. izd-vo Ministerstva oborony SSSR, 1955.
125 p. (MIRA 8:4)

(Matter) (Atomic energy)

~~KITAYGORODSKIY, A.I.~~; BOKIY, G.B., professor, otvetstvennyy redaktor;
~~SIRUCHKOV, Yu.T.~~, redaktor; MEVRAYNVA, N.A., tekhnicheskii re-
daktor

[Organic crystallochemistry] Organicheskaya kristallokhiimiya. Mo-
skva, Izd-vo Akademii nauk SSSR, 1955. 558 p. (MIRA 8:7)
(Crystallochemistry)

KITAYGORODSKIY, A.I.

USSR/ Chemistry - Physical chemistry

Card 1/1 Pub. 147 - 17/21

Authors : Kozhin, V. M., and Kitaygorodskiy, A. I.

Title : Low temperature investigation of the structure of aromatic compounds.
Part 3. Crystalline and molecular structure of naphthalin

Periodical : Zhur. fiz. khim. 29/1, 1897-1908, Oct 1955

Abstract : A complete structural investigation of naphthalin was made at -195° C. Three-dimensional series were formulated and the coordinates of atoms and atomic functions were compared for temperatures of -195° and -70° C. An analysis of the interatomic spaces showed that the contraction in the nucleus is due to the changes in the spaces between various molecules. Equalization of the intermolecular radii was observed during temperature drops. Five references: 4 USSR and 1 USA (1946-1953). Tables; diagrams.

Institution : Acad. of Sc., USSR, Inst. of Organoelemental Compounds, Moscow

Submitted : April 6, 1955

USSR/ Chemistry - Physical chemistry

Card 1/1 Pub. 147 - 14/22

Authors : Kozhin, V. M., and Kitaygorodskiy, A. I.

Title : Low temperature investigation of the structure of aromatic compounds.
Part 4. The anisotropy of thermal expansion in benzene

Periodical : Zhur. fiz. khim. 29/11, 2074-2075, Nov 55

Abstract : The anisotropy of thermal expansion in benzene was measured on benzene monocrystals by means of x-ray structural analysis. The dimensions of an elementary nucleus for temperatures of -20 and -195°C were established. The mean thermal expansion coefficients in the direction of the main thermal deformation axes of the benzene crystal were determined. It was found that an increase in the molecule per one benzene ring is connected with a constant ratio of mean volumetric values of the expansion coefficients. Six references: 2 USSR, 2 USA, 1 Germ. and 1 Ital. (1924-1954). Drawing.

Institution : Acad. of Sc., USSR, Inst. of Organoelemental Compounds, Moscow

Submitted : April 6, 1955

KITAYGORODSKIY, A. I.

USSR/ Chemistry - Crystallography

Card 1/1 Pub. 22 - 12/51

Authors : Kitaygorodskiy, A. I.

Title : The theory of determining signs of structural amplitudes

Periodical : Dok. Ak. Nauk SSSR 101/1, 73-76, Mar 1, 1955

Abstract : Experiments showed that the newly prepared theory of determining signs of structural amplitudes is based on the analysis of a certain expression. It is explained that the absolute value of structural amplitudes F can be found by studying the centro-symmetrical crystal by means of the x-ray analysis method. A formula is presented for the calculation of single structural amplitudes. Differences in the sign can be seen only in the case of faint reflections at a considerable deviation of the atom from the parallel lines. The numerical values of single structural amplitudes were found to be independent from each other. (Sight references: 5, 1954 and 5, English (1949-1954)).

Institution : Acad. Sci., USSR, Institute of Crystallography, Leningrad

Presented by : A. I. Kitaygorodskiy, U. V. Rylov, Moscow, U. S. S. R., 1954

KITAYGORODSKIY, A. I.

USSR/ Chemistry - Crystallography

Card 1/1 Pub. 22 - 26/62

Authors : Kitaygorodskiy, A. I.

Title : ~~New method of direct structural analysis of crystals~~

Periodical : Dok. AN SSSR 102/3, 519 - 520, May 21, 1955

Abstract : A new method of direct structural analysis of crystals is briefly described. The method makes it possible to establish the arrangement of atoms in the elementary nucleus of the crystal without any hypotheses regarding the structure of the crystal and without the need of structural models. Some results obtained by the new method are listed. One USSR reference (1955).

Institution : Acad. of Sc., USSR, Inst. of Elementorganic Compounds

Presented by: Academician N. V. Belov, February 15, 1955

USSR/Solid State Physics - Structural Crystallography, E-3

Abst Journal: Referat Zhur - Fizika, No 12, 1956, 34585

Author: Kitaygorodskiy, A. I.

Institution: Institute of Elementary Organic Compounds, Academy of Sciences USSR

Title: Theory of Connection Between Structural Amplitudes

Original Periodical: Dokl. AN SSSR, 1955, 105, No 3, 482-484

Abstract: General relationships are obtained between individual structural amplitudes. To derive the relationship, one introduces n linearly-independent vector of the type

$$G_p = \sum_{j=1}^N e_j n_j^{1/2} \exp 2\pi i H_p r_j$$

The scalar products of the vectors $G_p G_q^*$ is

equal to the single structural amplitude of the $H_p - H_q$ lattice point of the inverse lattice. Assuming that the vectors $G_1, G_2, G_3 \dots G_{m-1}$ are fixed and that the values of the structural amplitudes $F_{1,m}, F_{2,m}, \dots F_{m-2,m}$ are known, or what is the same, the cosines of the angles between the vectors G_1 and G_m ; G_2 and G_m ; ..., G_{m-2} and G_m are known, it is possible to explain the limitations that are imposed thereby on the position of the vector G_m . The relationship $F_{m,m-1} = A + B \cos \varphi$, is established,

1 of 2

- 1 -

USSR/Solid State Physics - Structural Crystallography, E-3

Abst Journal: Referat Zhur - Fizika, No 12, 1956, 34585

Author: Kitaygorodskiy, A. I.

Institution: Institute of Elementary Organic Compounds, Academy of Sciences USSR

Title: Theory of Connection Between Structural Amplitudes

Original Periodical: Dokl. AN SSSR, 1955, 105, No 3, 482-484

Abstract: where A and B are expressed in the terms of all the remaining specified Ppq. This relationship appears to be the most general. The known inequalities, relating the structural amplitudes, and also all the probability relationships, should follow from this relationship.

KITAYGORODSKIY, Aleksandr Isaakovich; GUROV, K.P., redaktor; KUZNETSOVA,
Ye.B., redaktor; TUMARKINA, N.A., tekhnicheskiy redaktor

[Order and disorder in the world of the atoms] Poriadok i besporiadok
v mire atomov. Izd. 2-oe, perer. i dop. Moskva, Gos. izd-vo tekhniko-
teoret. lit-ry, 1956. 138 p. (MIRA 10:2)
(Atoms)

KILAYGORODSKIY A.I.

Aug.

Category : USSR/Solid State Physics - Structural Crystallography E-3

Abs Jour : Ref Zhur - Fizika, No 3, 1957, No 6508

Author : Kilaygorodskiy, A.I.

Inst : Institute of Elementary Organic Compounds, Academy of Sciences, USSR.

Title : Kristallografiya, 1956, 1, No 1, 14-16

Abstract : On the basis of the theory of the connection between the structural amplitudes, developed by the author, plots are prepared for the determination of the reliably positive structural products $F_H F_K F_{K-H}$. Using the author's formula for the probability of the positive sign of the structural product, $P_+ = 1/(1 + \xi)$, where

$$\xi = \frac{\sqrt{1 - F_H^2 - F_K^2 - F_{K-H}^2 - 2|F_H F_K F_{K-H}|}}{F_H F_K F_{K-H}}$$

curves are plotted for the probability of the positive sign for structural products of different magnitude and of different dependence of $x = F_H F_K F_{K-H}$. It is established that

Card : 1/2

KITAYGORODSKIY, A. I.

USSR/ Chemistry - Molecular compounds

Card 1/1 Pub. 40 - 20/25

Authors : Kolesnikov, G. S.; Korshak, V. V.; Andreyeva, M. A.; and Kitaygorodskiy, A. I.

Title : High molecular compounds. Part 90. Polycondensation of 1,2-dichloroethane with tetralin

Periodical : Izv. AN SSSR. Otd. khim. nauk 1, 114-119, Jan 1956

Abstract : The polycondensation of 1,2-dichloroethane with tetralin was investigated in the presence of aluminum chloride and the basic laws governing this polycondensation process were established. On the basis of x-ray analysis it was determined that 1,2-di-(beta-tetralyl) ethane is the product obtained during the initial polycondensation stages. The formation of three-dimensional polycondensation products was observed in spite of the fact that the potential function of tetralin is only 4. The effect of benzene-solution concentrations of polytetralylenethyl on the polymer molecule association is discussed. Seven references: 5 USSR and 2 Germ. (1921-1955). Tables; graph.

Institution : Acad. of Sci., USSR, Inst. of Organoelemental Compounds

Submitted : November 18, 1954

KITAYGOREDSKIY, A.I., professor, doktor fiziko-matematicheskikh nauk.

Interesting facts on important things ("Time and its measurement."
P.S.Zavel'skii. Reviewed by A.I.Kitaigorodskii). Nauka i zhizn' 2)
no.9:60 '56. (Time measurements) (MLRA 9:10)

KITAYGORODSKIY, A.I., professor (Moskva)

In the world of physics ("Universe and atom." V. Mesentsev.
Reviewed by A.I. Kitaigorodskii. Priroda 45 no.2:119-120 P '56.
(Atoms) (MLBA 9:5)

KITAYGORODSKIY, A. Y.

Institute of Elemento-Organic Compounds, Moscow-"Theorie de Correlation entre les Facteurs de Structure et les Methodes Directes de l'Analyse de Structure" (Section 2-13); " Sur les Cristaux Mixtes de Composants Organiques" (Section 7-1); L'Empaquement de Molecules Longues" (Section 7-19) papers submitted at the General Assembly and International Congress of Crystallography, 10-19 Jul 57, Montreal, Canada.

C-3,800,189

KITAYGORODSKIY, A. Y., KHOTSYANOVA, T. L., and STRUCHKOV, G. T.

Institute of Elemento-Organic Compounds, Moscow: "The Crystal Structure of Some Tropylium Salts" (Section 7-11) a paper submitted at the General Assembly and International Congress of Crystallography, 10-19 Jul 57, Montreal, Canada.

C-3,800,189

RESEARCH INSTITUTE, A. S.

"X-ray investigation of linear polyethers," a paper presented at the 9th Congress on the Chemistry and Physics of High Polymers, 20 Jan-2 Feb 57, Moscow. Research Inst. for Organic Chemistry, AD USSR.

2-3,004,325

Kitaygorodskiy, A.I.

NUCLEAR TECHNOLOGY AND APPLICATIONS: POPULAR SURVEYS

Structure of Matter and Its Energy, by Professor A. I. Kitaygorodskiy.
Second, corrected and supplemented edition; Moscow: Military Publishing
House of the Ministry of Defense USSR, 1957. 200 pages, 5 x 8 inches.

A popular book, apparently intended for people untrained in chemistry and physics. The table of contents follows: "Introduction;" "Structure of matter;" "Convenient measurement units;" "Atoms;" "Molecules;" "Various types of atoms of a chemical element;" "Decaying atoms;" "Three states of matter;" "Crystals;" "Invisible movements;" "Measurement of interatomic distances;" "Structure visible to the aided eye;" "Energy of matter;" "Mechanical energy and heat;" "Transformations of molecules;" "Chemical energy;" "Nuclear energy: collisions of atomic nuclei; artificial atoms; is it possible to obtain heat during nuclear transformations? nuclear fuel; operating principle of the atom bomb; operating principle of the nuclear reactor; constructions of nuclear reactors; soviet nuclear reactors; breeder reactors; problem of heat removal; protection against

Card: 1/2

KITAYGORODSKIY, Aleksandr Isaakovich; VAYNSHTEYN, B.K., doktor fiziko-matem.nauk,
otvetstvennyy red.; SHWIDY, V.V., red.isdatel'stva; ASTAF'YEVA, G.A, tekhn.red.

[A theory of structural analysis] Teoriia strukturnogo analiza.
Moskva, Izd-vo Akad.nauk SSSR, 1957. 283 p. (MIRA 10:12)
(Crystallography, Mathematical)

KLITYGORODSKIY, A. I.
KITAYGORODSKIY, A. I.

The structure of high polymers. Usp. khim. i tekhn. polim. no. 2:191-
201 '57. (MIRA 11:1)

(Polymers) (Molecular structure)

AUTHOR: Kitaygorodskiy, A.I.

70-3-5/20

TITLE: Theory of the correlation between the structural factors and the methods of direct analysis of the crystal structure. (Teoriya svyazi strukturnykh amplitud i metody pryamogo analiza struktury kristallov)

PERIODICAL: "Kristallografiya" (Crystallography), 1957, Vol. 2, No.3, pp. 352 - 357 (U.S.S.R.)

ABSTRACT: The law of predominant positivity of $F_H F_K F_{H+K}$ has been elucidated, a new method of its use for direct structure analysis being proposed. It has been demonstrated that statistical theories are of secondary importance both for proving and applying this law.

A very interesting rule can be deduced experimentally, namely: the structural product $X_{HK} = F_H F_K F_{H+K}$ is positive in most cases; the larger the absolute value of the structural product the larger will be the positive part of X_{HK} . The first definition of this law was given by this author in 1953 (4); he has shown that the law can be deduced on the assumption of a uniform distribution of the arguments of trigonometric functions which enter into the formulae of the structural factors. With this assumption, it is possible to

Card 1/7

70-3-5/20

Theory of the correlation between the structural factors and the methods of direct analysis of the crystal structure.
(Cont.)

determine the function of probability of the value X_{HK} and thus to show that it has a maximum value in the positive range. In the mentioned earlier work, it was shown that the possibility of a positive sign of the structural product can be expressed by:

$$W_+ = (1 + \exp [-2NX_{HK}])^{-1},$$

where N is the effective number of atoms on the lattice. Such a theory can be referred to as a statistical theory and it enables explanation of the predominance of the positive value of X_{HK} and the fact that statistical ideas should be the basis of direct methods of structural analysis. By a more detailed study, the author shows that this view is erroneous; statistical theories have a predominance rule only in the case of small X_{HK} values. For large X_{HK} values (and only large values have any practical interest) the law of predominance of the positive value of X_{HK} has a completely different and

Card 2/7

70-3-5/20

Theory of the correlation between the structural factors and the methods of direct analysis of the crystal structure.
(Cont.)

This determinant can be written in the form of a well-known series and we thus obtain:

$$1 - \sum_H P_H^2 + \sum_{H,K} P_H P_K P_{H+K} - \dots > 0.$$

The here written terms are the most important of the sum. It is obvious that the positive value of the sum can be obtained only if the largest part of the structural products are positive. This formula shows that all the structural products, without exception, will be positive if the values of P composing the determinant exceed a certain limit δ . Thus, the direct method of determination of the signs of the structural factors is based on the property of the determinant D and not on the ideas of statistical distribution of the atomic co-ordinates in the lattice. The predominance of the positive values of large structural products does not correspond to any statistical theory whatever. If the structural product is not an absolute positive value the question of probability of its positive sign can be discussed. Inaccurate formulation and ignoring the absolute correlations between the factors has led various authors to

Card 4/7

70-3-5/20

Theory of the correlation between the structural factors and the methods of direct analysis of the crystal structure.
(Cont.)

calculating the probability density of the structural product instead of calculating the probability of the structure for which the structural product has a given value. The expressions for the probability of the sign being positive for X_{HK} deduced in previous work does not indicate the existence of any critical value of X when the probability is reduced to one. The correct expression for the probability of the positive sign of the structural product is $W_+ = 1/(1 + \epsilon)$, where

$$\epsilon = \sqrt{\frac{1 - F_H^2 - F_K^2 - F_{K+H}^2 - 2F_H F_K F_{K+H}}{1 - F_H^2 - F_K^2 - F_{K+H}^2 + 2F_H F_K F_{K+H}}} \times \exp[-2N \cdot F_H F_K F_{K+H}].$$

Card 5/7 The author believes that formulae of statistical origin are of secondary importance. The direct methods which permit finding the signs of the structural factors are effective only in the case where a large number of structural products have definitely

70-3-5/20

Theory of the correlation between the structural factors and the methods of direct analysis of the crystal structure.
(Cont.)

a positive sign. The good results obtained by the direct method are not at all linked with statistical theories. The author believes that work with direct methods should be effected by composition of all types of D_m determinants. The correct signs of the structural factors should not give a negative value to any determinant. It is shown that the rule: $X_{HK} > 0$ if $|X_{HK}| > -1/8$ can be extended to determinants of any order. If the determinant of the order m is composed of F for which $|F| > 0_m$, all the structural products which do not enter into the determinant are definitely positive. The magnitudes of a_m decrease with increasing m . Analysis

of the determinants of high orders permits judgment of the positivity of a structural product one hundred times smaller than $1/8$. The author believes that the method which permits direct determination of the signs of the structural factors will play an important role in X-ray structural analysis. However, for this purpose, the use of computers is indispensable.

Card 6/7

Kitaygorodskiy, A.I.

70-4-2/16

AUTHOR: Kitaygorodskiy, A.I.

TITLE: Ideas relating to organic crystallo-chemistry (Idea
organicheskoy kristallokhimii)

PERIODICAL: "Kristallografiya" (Crystallography), 1957,
Vol.2, No.4, pp. 456 - 465 (U.S.S.R.)

ABSTRACT: The thermodynamical aspect of the theory of close packing of molecules in crystals is discussed and new applications are considered of the theory for the purpose of deriving the possible structures of paraffin crystals, as well as establishing the conditions involved in the formation of solid solutions.

The ideas of the author relating to the symmetry and the density of packing of molecules in a crystalline system enabled formulation of the following rules of formation of maximum organic crystals: 1) the solutions of "interclusion" can form only if the volumes of the molecules are in the ratio (8 to 10): 1; 2) substitution solutions always exist when the configurations of the molecules forming the mixture are sufficiently near to each other; 3) mixed crystals can form at any ratios under the above mentioned conditions only if the packing symmetry of the molecules (spatial group and number of molecules in the lattice) is equal for the individual components.

Card 1/3

70-4-2/16

Ideas relating to organic crystallo-chemistry. (Cont.)

inside the crystal. From this and from the last mentioned rule, it can be seen that molecules like those of naphthalene or anthracene cannot constitute a continuous series of solutions with mono-derivatives. Most of the data concerning continuous series disagree with the above mentioned condition and therefore one must conclude that these data are erroneous. For verifying the above mentioned rules, the author studied the systems dibenzyl-stilbene, phenanthrene-anthracene and anthracene. Data of published work indicate that these components form a continuous series of solutions. The above mentioned third rule indicates, however, that such continuous solutions cannot exist. In the three cases mentioned, the author obtained perfect crystals of mixtures of each composition; the diffraction diagrams established by means of Weissenberg goniometer have shown that the here mentioned rule is correct and that the previous experimental results were erroneous. The studied systems have diagrams of state with a eutectic and a peritectic. Substitution of the molecules is absolutely irregular. The entry of one molecule of a different substance in the crystal is controlled solely by the law of close packing. This indicates that the foreign molecule chooses such a position in which the intra-molecular distances differ as slightly as

Card 2/3

Card 3/3

AUTHOR: Kitaygorodskiy, A.I.

70-5-13/31

TITLE: The Packing of Chain Molecules (Upakovka tseposhechnykh molekul) II. Layers of Paraffin Molecules (II. Sloi molekul parafinov)

PERIODICAL: Kristallografiya, 1957, Vol.2, No.5, pp. 646-652 (USSR)

ABSTRACT: On the basis of the theory of the close-packing of molecules (see Organicheskaya Kristallokhimiya, 1955 by A.I. Kitaygorodskiy) the possible symmetries and dimensions of layers of paraffin molecules are deduced. Three pseudocells are first distinguished R-orthorhombic with $a_0 = 4.96$, $b_0 = 7.42$ and $c_0 = 2.54$ Å; M-monoclinic with $a_0 = 4.2$, $b_0 = 4.4$, $c_0 = 2.54$ Å and $\gamma = 111^\circ$; T-triclinic with $a_0 = 4.3$, $b_0 = 4.8$, $c_0 = 2.54$ Å and $\alpha = 90^\circ$, $\beta = 108^\circ$, $\gamma = 107^\circ$. m is a whole number, $c_0 = 2.54$ Å is the distance between two methylene groups so that the identity distance parallel to c_0 is mc_0 Å. m is the displacement of the molecule parallel to the a-axis and n parallel to the b-axis. The two-dimensional layer cell is determined by the pseudo-cell and by m and n . Each pair of numbers m and n give

Ch 11/3

70-5-13/31

The Packing of Chain Molecules. II. Layers of Paraffin Molecules.

four layers: $m, n; \bar{m}, \bar{n}; \bar{m}, n; m, \bar{n}$. The possible layers are tabulated: T-pseudocell - the ab plane of the layer coincides with the a_0b_0 plane of the pseudocell and the symbols are $T(1/2, 0)$ and $T(-1/2, 0)$. Each molecule has 6 neighbours. M-pseudocell - besides the rectangular layer $M(0, 0)$ there are oblique layers $M(1, 0), M(-1, 0), M(0, 1)$ and $M(0, -1)$. R-pseudocell - besides the rectangular layer $R(0, 0)$ there are oblique layers $R(0, 1), R(0, -1); R(1, 0)$ and $R(-1, 0)$ and four layers with m and n equal $R(1, 1), R(1, -1), R(-1, 1)$ and $R(-1, -1)$. The geometrical parameters of these layers are tabulated (cell edges and angles). The symmetry of the layers is determined not only by the geometrical parameters but also by the symmetry of the particular molecules. If the paraffin chain has an even number of C atoms, then its symmetry is $2/m$ if an odd number, then mm . The various combinations of symmetry are tabulated diagrammatically. There are 3 figures, 1 table and 4 references, 1 of which is Slavic.

ASSOCIATION: Institute of Elemental-organic Compounds.
Card 2/3 (Institut Elementoorganicheskikh soyedineniy)

70-5-13/31

2. Packing of Chain Molecules. II. Layers of Paraffin Molecules.

RECEIVED: May 15, 1957.

AVAILABLE: Library of Congress

100 3/3

KITAYGORODSKIY, A.I.
APPROVED FOR RELEASE: 09/17/2001

CIA-RDP86-00513R000722920003-6

AUTHOR: None Given.

TITLE: General Meeting of the Department for Chemical Sciences of the AN USSR Held in May 30-31 and June 28, 1957 (Obshchiye sobraniya Otdeleniya khimicheskikh nauk Akademii nauk SSSR 30-31 maya i 28 iyunya 1957 g).

PERIODICAL: Izvestiya AN SSSR, Otdel. Khim. Nauk, 1957, Nr 11, pp. 1416-1419 (USSR)

ABSTRACT: Chairman: Member of the Academy A. P. Vinogradov.
Lectures: A. N. Terenin, Member of the Academy.
"Spectroscopy of the Molecular Compounds with Metal Halides."
V. N. Filimonov, the student D. Borsovy and Sh. Sh. Raskin helped the author in his work.
S. Z. Roginskiy, corresponding Member of the Academy,
B. V. Nekrasov, corresponding Member of the Academy,
N. D. Sokolov, Doctor of chemical sciences, M. M. Shenvakin, corresponding Member of the Academy, A. I. Kitaygorodskiy, Doctor of physico-mathematical sciences, A. P. Vinogradov, Member of the Academy, took part in the discussion.
B. P. Nikol'skiy, corresponding Member of the Academy of

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APPROVED FOR RELEASE: 09/17/2001

CIA-RDP86-00513R000722920003-6"

KITAYGORODSKIY, A.I., doktor fiziko-matematicheskikh nauk.

First book on the subject ("Structural electronography" by B.K. Vainshtein. Reviewed by A.I. Kitaigorodskii). Vest.AN SSSR 27 no.4: 136-138 Ap '57. (MLRA 10:5)
(Electron diffraction examination)
(Vainshtein, B.K.)

AUTHOR
TITLE

KITAYGORODSKIY A.I.

PA - 3156

The Conditions for the Formation of Organic Solid Solutions.
(Usloviya obrazovaniya tverdykh rastverev organicheskikh veshch-
estv -Russian)

PERIODICAL

Doklady Akademii Nauk SSSR, 1957, Vol 113, Nr 3 pp 664-666 (U.S.S.R.)

Received 6/1957

Reviewed 7/1957

ABSTRACT

The attempt was made to determine the correlation between the amount of solubility and the dimensions of the cavities and bulges formed on the occasion of mixing. Dissolution by penetration is possible only in the rarest of cases in organic systems. The packing coefficients of the organic molecules in the crystal are within range of from 0,6 to 0,8. This means that in organic crystals only small cavities are possible. These cavities have a total volume of 10% of the molecular volume. Thus, solid solutions can be formed when A penetrates into B only if the molecules of A are about ten times smaller, with respect to volume, than those of B. It stands to reason that not only the volume but also the shape of the cavities is of importance. If the molecules of A and B are more or less equal with respect to size and shape, the molecules of A are able to replace those of B in the crystal. The symmetry of molecular distribution in the crystal changes abruptly as soon as the first molecules of A enter the solution, if the molecules of B are not asymmetric, but if those of A are asymmetric

Card 1/2

Card 2/2

"APPROVED FOR RELEASE: 09/17/2001

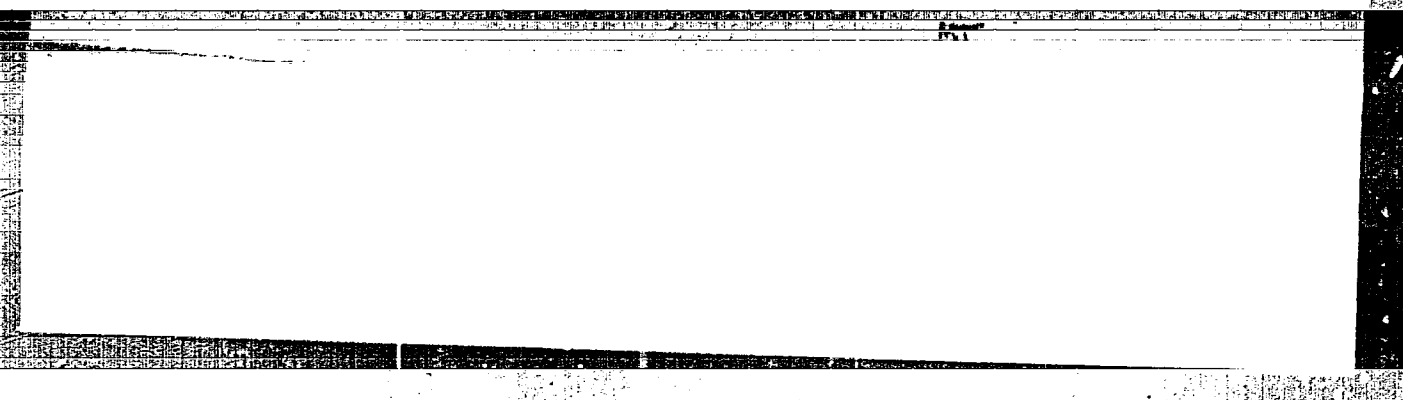
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CIA-RDP86-00513R000722920003-6



APPROVED FOR RELEASE: 09/17/2001

CIA-RDP86-00513R000722920003-6"

KITAYGORODSKIY, A. I.

"Some Physical Problems of Organic Crystals."

report presented at the Conf. on Mechanical Properties of Non-Metallic Solids, Leningrad, USSR, 19-26 May 1958.

Inst. of Elemento-Organic Compounds, Moscow.

CHAYKIN, A. T., A. S. ADEMANOV, I. V. KOSHLAKOVA, M. V. VOL'KOVICH

"Defective Crystalline States."

report presented at the Conference on Investigation of Mechanical Properties of
Non-Metals, by the Intl. Society of Pure and Applied Physics and the AS USSR,
at Leningrad, 19-24 May 1958.
(Vest. Ak Nauk SSSR, 1958, no. 9, pp. 109-111)

KITAYGORODSKIY, A. I.

A. I. Kitaygorodskiy and Yu. T. Struchkov, "Conformations of Molecules of Sterically Stretch Benzene Polyderivatives."

report presented at the Symposium on Concepts of Conformation in Organic Chemistry which took place in Moscow at the IOKh AN SSSR (Institute of Organic Chemistry, AS USSR) from September 30 to October 2, 1958.

Izvestiya Akademii nauk SSSR, Otdeleniye khimicheskikh nauk, 1959, No. 3, 561-564.

5(3)

PHASE I BOOK EXPLOITATION

SOV/1405

Kitaygorodskiy, Aleksandr Isaakovich

Struktura polimerov (Structure of Polymers) Moscow, Izd-vo
"Znaniye," 1958. 28 p. (Series: Vsesoyuznoye obshchestvo
po rasprostraneniyu politicheskikh i nauchnykh znaniy.
Seriya VIII, 1958; vyp. II, no. 21) 48,000 copies printed.

Sponsoring Agency: Vsesoyuznoye obshchestvo po rasprostraneniyu
politicheskikh i nauchnykh znaniy.

Ed.: Faynboym, I.B.; Tech. Ed.: Berlov, A.P.

PURPOSE: This book is intended for persons engaged in textile
manufacturing, biological research, structural engineering or
any field where polymers or high-molecular compounds are of
interest.

Card 1/2

Structure of Polymers SOV/1405

COVERAGE: The book explains the structure and mechanism of formation of high-molecular compounds as a basis for determining the properties of plastics and artificial fibers and the structure of proteins and other biologically important substances which may explain the biochemical and biological behavior of test subjects. Diagrams and drawings of bond distribution, atomic arrangements and crystal orientation are given. The following new theory of the structure of polymers by V.A. Kargin, A.I. Kitaygorodskiy and G.L. Slonimskiy is discussed: a polymeric substance is thought to consist of non-entangling bundles of long-chain molecules, molecules of different length (weight) constituting the same bundle as if following each other. Other such molecules constitute neighboring chains, which maintain their position throughout the bundle. A bundle may shift its direction as a whole in patterned (regular) fashion. By this regular shifting, all molecules lie in the same plane.

CONTENTS:

Chemical Structure	3
The Structure of Molecules	7
The Structure of a Polymeric Substance	15

AVAILABLE: Library of Congress

Card 2/2

TM/bj
4-29-59

AUTHORS: Myasnikova, R.M. and ~~Kitaygorodskiy, A.I.~~ 70-3-2-5/26

TITLE: The Structures of Mixed Crystals of the System Acridine-Anthracene (Stroyeniye smeshannykh kristallov sistemy akridin-antratsen)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 2, pp 160 - 166 (USSR).

ABSTRACT: The anthracene and acridine molecules are geometrically similar but owing to the presence of a nitrogen atom in the acridine molecule, their symmetries are mmm and $mm2$ respectively. It was earlier thought that a continuous range of solid solutions is formed but this is shown to be incorrect and that there are breaks at 4% and 28% anthracene. From 0- 4.6% anthracene needle crystals are formed; between 4.6 and 28.2% monocrystals were not formed and at greater concentrations plates were produced. The unit cell dimensions were: 100% acridine $a \cdot \sin \beta = 16.35$, $b = 18.51$, $c = 6.07 \text{ \AA}$, packing coefficient $k = 0.713$; 4.6% anthracene $a \cdot \sin \beta = 17.08$, $b = 19.60$, $c = 6.08$, $k = 0.644$; 28.2% anthracene $a = 8.421$, $b = 6.06$, $c = 11.054$, $\beta = 123^\circ 46'$, $k = 0.707$; 100% anthracene $a = 8.561$, $b = 6.036$, $c = 11.163$, $\beta = 124^\circ 42'$, $k = 0.722$. At the anthracene-rich end there are 2 molecules per unit cell and at the other end 8 molecules.

Card 1/2

The Structures of Mixed Crystals of the System Acridine-Anthracene ^{70-3-2-5/26}

There are 4 figures, 2 tables and 6 references, 3 of which are Soviet and 3 English.

ASSOCIATION: Institut elementoorganicheskikh soedineniy AN SSR
(Institute of Elemental-organic Compounds, Ac.Sc. USSR)

SUBMITTED: July 9, 1957

Card 2/2

KITAYGORODSKIY, A. I.

70-3-2-24/26
AUTHORS: Belov, S.V., Belozyor, L.N., Bely, S.B., Brumkhova, Ye.G.,
Vaynshteyn, S.E., Zhidnev, S.M., Zhurav, V.I., Kitagorod-
skiy, A.I. and Plachov, S.V.
TITLE: The Fourth International Congress of Crystallography
(IV mezhnatsionnyy kongress kristallografov) (Montreal,
July 10-19, 1977)
PERIODICAL: Kristallografiya, 1978, Vol 3, No 2, pp 250 - 260
(USSR).
ABSTRACT: Outline of the scientific proceedings of the
conference.
Card 1/1

000000-00-44577

AUTHORS: Kitaymorodskiy, A.I., Mnyukh, Yu.V. and Nechitaylo, N.A. 70-3-3-7/36
 TITLE: An Investigation of Solid Solutions of Certain n-paraffins
 (Issledovaniye tverdykh rastvorov nekotorykh n-parafinov)
 PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 3, pp 298 - 303
 (USSR).

ABSTRACT: X-ray and thermographic analysis of the binary systems formed from the paraffins with C_{18} , C_{19} and C_{20} were made. Regularities followed from the theory of close packing of molecules were established and an orthorhombic phase was found in $C_{18} - C_{20}$. In identical conditions the solubility of molecules with longer chains is less than that of molecules with shorter chains. The theoretical conclusion on the impossibility of a continuous range of solid solutions in mixtures of odd and even paraffins was confirmed. X-ray powder photographs were taken at room temperature and at temperatures from $-100^{\circ}C$ up to the melting points. It was found that in the systems $C_{18} - C_{19}$ and $C_{20} - C_{19}$ there was no continuous range of solid solutions. The $C_{18} - C_{20}$ system also showed no continuous range of solid solutions in spite of the isomorphism of the crystals $C_{18}H_{38}$ and

Card1/2

70-3-3-7/36

An Investigation of Solid Solutions of Certain n-paraffins

$C_{20}H_{42}$ which are tri-clinic with very similar dimensions.

The region from 8% C_{20} to 81% C_{20} was orthorhombic.

Phase diagrams of the systems $C_{12} - C_{13}$, $C_{13} - C_{14}$ and $C_{14} - C_{15}$ are given. The increased solubility of shorter

molecules in a given solvent is explained by the lesser disturbance to the structure caused by holes in the structure compared to that caused by extra groups intruding.

There are 5 figures and 9 references, 6 of which are Soviet, 2 English and 1 French.

ASSOCIATION: Institut elementoorganicheskikh soedineniy, Institut nefti (Institute of Elemento-organic Compounds. Oil Institute)

SUBMITTED: December 4, 1957.

Card 2/2

AUTHOR: Kitaygorodskiy, A.I.

70-3-3-34/36

TITLE: On the Impossibility of Distributing Centre-symmetrical Molecules in Non-centrosymmetrical Groups (O nevozmozhnosti razmeshcheniya tsentrosimmetrichnykh molekul v netsentrosimmetrichnykh gruppakh)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 3, pp 391 - 392 (USSR)

ABSTRACT: A statement by Gerbstein and Schönning (Acta Crystallogr., Vol 10, p 657, 1957) that centrosymmetric molecules can form crystals without a centre of symmetry is contested. Two cases are examined: 1) The number of molecules is equal to the multiplicity of the general position in the group. The group $P2_1$ is used as an illustration, the contention being demonstrated for this case. In the case 2) the number of molecules is greater than the multiplicity of the general position and not all molecules are identically situated. Here, centrosymmetrical molecules must associate into non-centrosymmetrical groups; this contradicts principles set out by Kitaygorodskiy in his book "Organicheskaya kristallografiya". The four examples which Gerbstein and Schönning quote are criticised as being of definite space group but uncertain centrosymmetry of

Card 1/2

70-3-3-34/36

On the Impossibility of Distributing Centrosymmetrical Molecules in
non-centrosymmetrical Groups

the molecules. For mercury ethyl mercaptan, only the positions of the heavy atoms were determined. Difluorenylidene is more doubtful and steric hindrance may make the fluorene nucleus non-planar. In 4, 4'-dinitrodiphenyl steric hindrances due to the ortho atoms of hydrogen disturb the planarity. 1,2,5,6-dibenzanthracene exists in two modifications, the α -modification being centrosymmetrical and the β assumed non-centred. This assumption is contested. The β is thought to be a cis-form and the α a trans-form.

There are 2 Soviet and 1 English references.

ASSOCIATION: Institut elementoorganicheskikh soedineniy
(Institute of Elemental - Organic Compounds)

SUBMITTED: December 27, 1957
Card 2/2

AUTHOR: Kitaygorodskiy, A. I., Doctor of Physical and Mathematical Sciences 30V/30-58-6-4/45

TITLE: The Problem of the Structure of High-Molecular Substances
(Problema stroeniya vysokomolekulyarnykh veshchestv)

PERIODICAL: Vestnik Akademii nauk SSSR, 1958, ²¹№ 6, pp. 35 - 42 (USSR)

ABSTRACT: Synthetic materials, synthetic fibers, cellulose, albuminous substances, give an idea of the place taken by high-molecular substances in modern engineering and biology. According to the author's opinion, the investigators face two tasks: the first consists in finding common rules governing the structure of such substances as linear polymeric compounds and globular albuminous substances; the second consists in the development of detailed methods of the structural characteristic of individual substances. Only 2 classes of high-molecular compounds can at present be discussed from the general point of view - linear polymeric compounds, as well as globular protein. Moreover, the author explains his proposal for the solution of the structural problem of linear polymeric com.

Card 1/4

The Problem of the Structure of High-Molecular Substances

304/30-58-6-4/45

pounds. This problem consists in the problems of the structural investigation of both individual molecules and molecule-conglomerates. The structural investigation of the elements of which the albumin molecules consist, ought to precede the investigation of the albuminous structures. Concerning the production of high-molecular materials with the properties required, the problems of reciprocal arrangement of the molecules do not play a smaller part than the problems connected with the structure of an individual molecule. The author refers here to his previous work which he carried out in collaboration with V. A. Kargin and G. L. Slonimskiy (Ref 1). Regarding the problems of organic crystal chemistry, the author refers to his previous work (Ref 2). Concerning the problem of the tensions between the molecules, the author refers to the work by V. A. Kargin and G. L. Slonimskiy (Ref 3). With respect to the globular proteins, the determination of the form and the dimensions was achieved for a great number of objects. Furthermore, the author gives a relative characteristic of the physical methods of the structural investigation of high-molecular substances. The author considers the working out of a method for the detailed characteristic of the

Card 2/4

The Problem of the Structure of High-Molecular Substances

30V/ 30-58-6-4/45

degree of order of the molecules in polymeric compounds to be one of the most important problems in the field of the structure of high-polymeric substances. The author further found out that the investigations in the field of the structure of high-polymeric substances in the Soviet Union are not carried out with the necessary impetus. He regrets that nobody is occupied with the structural investigation of globular albuminous substances by means of diffraction methods which are of greatest importance for biology. The author is satisfied that the first steps in the field of the investigation of albuminous substances were carried out by means of the electron-resonance-method. He also finds backwardness in the field of albumin-radiography. According to his opinion, at least 2 research centers for albuminous structure ought to be established. In the field of the investigation of synthetic fiber and other high-polymeric substances it looks much better due to the systematic work carried out by V. A. Kargin and his collaborators, but also here he states the lack of a corresponding laboratory. The

Card 3/4

The Problem of the Structure of High-Molecular Substances SOV/ 30-58-6-4/45

Laboratory of the Institute of High-Molecular Compounds, AS USSR in Leningrad, is under construction at present and cannot meet all requirements. The existing laboratories for the investigation of synthetic materials must be reinforced. There are 4 references, 3 of which are Soviet.

1. Synthetic materials--Structural analysis
2. Synthetic materials--Development
3. Molecular structure--Analysis

Card 4/4

AUTHORS: Kitaygorodskiy, A. I., Mnyukh, Yu. V. S07/20-121-1-31/55

TITLE: A Triclinic Modification of Polythene (Triklinnaya modifikatsiya politena)

PERIODICAL: Doklady Akademii nauk SSSR, 1958, Vol. 121, Nr 1, pp. 115-116 (USSR)

ABSTRACT: 1) Molecules of the paraffin type may crystallize either in a triclinic (T), monoclinic (M), or rhombic (R) form (Ref 1). Triclinic subcells were found in normal paraffins with an even atomic number of carbons from C₁₈ to C₂₆ and in some normal sebacoic acids, and others, whereas rhombic were found in the case of polythene and other straight paraffins of C₂₀ and in the case of some normal sebacoic acids. Substances with monoclinic subcells have hitherto not been found. The difference in free energy between the packing R and T is not great. Even several percents of admixtures of adjacent homologues cause the transformation of the triclinic structure of an n-paraffin to a rhombic one. The packing in the T-subcell has the highest density of all possible packing types, the R-subcell has, however, a higher symmetry. The probable existence

Card 1/3

A Triclinic Modification of Polythene

SOV/20-121-1-31/55

of the triclinic polythene modification was already earlier pointed out on the strength of the analysis of the packing of long chain molecules (Ref 4). 2) As far as the T-subcell has a high coating density we may assume that this strength is possible only in polythene samples with perfect structure, i.e. the cleanest and with a minimum number of side ramifications. A Debye-Scherrer X-ray diagram gave an image which is characteristic of a two phase system R + T. The modification occurred in a smaller quantity than the rhombic one. Figure 1 shows the last mentioned X-ray diagram and another one for the phase diagram of n-paraffins (Ref 5). The measurement of interplanar spacings and the comparison of the intensities confirmed finally the existence of the triclinic modification of polythene under normal conditions (Table 1). If the obtained results are compared with the data from the investigation of the n-paraffin C₃₀ under high pressure (personal note of S. S. Kabalkina and L. F. Vereshchagin) a second phase is detected beside the rhombic one (Table 1) in n-C₃₀. Thus the existence of the triclinic polythene modification which was assumed earlier by the authors was proved. There are 1 figure, 1 table, and 6 references, 4 of which are Soviet.

Card 2/3

A Triclinic Modification of Polythene

SOV/20-121-1-31/55

ASSOCIATION: Institut elementoorganicheskikh soedineniy Akademii nauk SSSR
(Institute of Elementary Organic Compounds AS USSR)

PRESENTED: March 1, 1958, by V. A. Kargin, Member, Academy of Sciences,
USSR

SUBMITTED: February 28, 1958

1. Methanes--Crystallization
2. Methanes--Molecular structure
3. Methanes--X-ray analysis

Card 3/3

AUTHORS: Kitaygorodskiy, A. I., Mnyukh, Yu. V. SOV/20-121-2-27/53

TITLE: The Variation of the Intermolecular Distances in Paraffin $n\text{-C}_{30}\text{H}_{62}$ With Temperature. Refining of the Molecule Form of the Paraffins (Temperaturnyye izmeneniya meshmolekulyarnykh rasstoyaniy v parafine $n\text{-C}_{30}\text{H}_{62}$. Utochneniye formy molekuly parafinov)

PERIODICAL: Doklady Akademii nauk SSSR, 1958, Vol 121, Nr 2, pp. 291 - 294 (USSR)

ABSTRACT: In the present paper a report is given on investigations of the subcells of normal paraffins. 2 forms of such subcells are known: The orthorhombic cell (R) and the triclinic (T) one (Refs 1,2). The purpose of the investigations was to explain details of the structures and to determine the distances between the separate H-molecules. The investigation was limited to: $n\text{-C}_{30}$ -paraffin (R-subcells), $n\text{-C}_{18}$ -paraffin (T-subcells), normal fatty acids (basic pattern of the packing as in normal paraffin, but steric hindrance because of the COOH -group, therefore packing frequently diverging from paraffin), penta decanoic

Card 1/3
7

SOV/20-121-2-27/53

The Variation of the Intermolecular Distances in Paraffin $n\text{-C}_{30}\text{H}_{62}$ With Temperature. Refining of the Molecule Form of the Paraffins

acid (T-subcells with $a=5,01 \text{ \AA}$ and $b=4,25 \text{ \AA}$), and iodoform ($J_1 - J'_1 = 3,98 \text{ \AA}$, $J_2 - J'_2 = 4,34 \text{ \AA}$). For $n\text{-C}_{30}$ -paraffin was obtained:

Distance between	(+52°)	(+20°)	extrapolated to -273°
$H_1 - H_3$	2,53	2,48	2,34
$H_1 - H_4$	2,95	2,92	2,86
$H_2 - H_4$	2,92	2,86	2,74
$H_2 - H_5$	2,43	2,42	2,36

There are 4 figures, 1 table, and 7 references, 4 of which are Soviet.

ASSOCIATION: Institut elementoorganicheskikh soedineniy Akademii nauk SSSR
(Institute of Elemental Organic Compounds, AS USSR)

Card 2/1
✓

AUTHOR: Gonikberg, M. G., Kitaygorodskiy, A. I. SOV/20-122-2-18/42

TITLE: On the Influence of Pressure Upon the Rate of Sterically Inhibited Reactions (K voprosu o vliyanií davleniya na skorent' prostranstvenno zatrudnennykh reaktsiy)

PERIODICAL: Doklady Akademii nauk SSSR, 1958, Vol 122, Nr 2, pp 231 - 234 (USSR)

ABSTRACT: The scarcely available experimental evidences suggest a considerable acceleration of the sterically inhibited reactions under increased pressure. Thus, tetramethyl ethylene was totally polymerized within 3 hours at 23,000 atmospheric excess pressure and at 300° whereas at 200° atmospheric excess pressure this was possible for 20% only. (Ref 1). The pressure also accelerates the thermal transformations of tetrachloro-ethylene at 300° and leads to the formation of hexachloro-butadiene and hexachloro-ethane (Ref 2). In both of these cases, the acceleration of reaction is but little related with the increasing concentration of the initial material. It is, however, caused by an increased velocity constant of the reaction by the

Card 1/4

On the Influence of Pressure Upon the Rate of
Sterically Inhibited Reactions

SOV/20-122-2-15/42

increase of pressure. In the present paper only the values $\Delta v_{\text{mol}}^{\ddagger}$ are discussed (change in volume of the reactive molecules at the formation of the activated complex). Obviously, this value is an essential component of the quantity

Δv^{\ddagger} . The authors confine their discussion to the reactions of Menshutkin which, by the way, were the object of various kinetic investigations at high pressure. They proceed from the conception of the structure of an activated complex as it is seen from the scheme (Fig 1, Ref 5). Then, reactions with pyridine, trimethylamine, and dimethylaniline are discussed. The values computed according to the scheme ($-\Delta v_{\text{mol}}^{\ddagger}$) reach some dozens cm^3 pro mol

for some Menshutkin reactions. With increasing pressure, this must lead to a considerable acceleration of these reactions according to the equation

Card 2/4

On the Influence of Pressure Upon the Rate of
Sterically Inhibited Reactions

SOV/29-122-2-10/42

$$\left(\frac{d \ln K}{dp} \right)_T = - \frac{\Delta v^\ddagger}{RT} \quad (1).$$

By the results of table 1 it becomes evident that the acceleration really occurs. The qualitative determination of a sterically inhibited formation process of an activated complex makes it possible to explain the various accelerations of the Menshutkin reactions by pressure if these reactions differ by the structure of the participating amines and haloid alkyls. In particular, the increasing acceleration of these reactions with the transition of CH_3J to $\text{C}_2\text{H}_5\text{J}$ and to $\text{iso-C}_3\text{H}_7\text{J}$ as well as of $\text{C}_5\text{H}_5\text{N}$ to $(\text{CH}_3)_3\text{N}$ and to $\text{C}_6\text{H}_5\text{N}(\text{CH}_3)_2$ becomes clear, further the same pressure effect in the reactions of trimethylamine and triethylamine. Of course, for a perfect analysis of the influence of pressure upon the velocity of the reaction, all Δv^\ddagger are to be considered. There are 3 figures, 1 table, and 11 references, 3 of which are Soviet.

Card 3/4

On the Influence of Pressure Upon the Rate of
Sterically Inhibited Reactions

SOV/26-122-2-16/42

ASSOCIATION: Institut organicheskoy khimii im.N.D.Zelinskogo Akademii nauk
SSSR (Institute of Organic Chemistry imeni N.D.Zelinskiy, AS USSR)

Institut elementoorganicheskikh sovedineniy Akademii nauk SSSR
(Institute of Elementary Organic Compounds, AS USSR)

PRESENTED: April 29, 1958, by B.A.Kazanskiy, Member, Academy of Sciences,
USSR

SUBMITTED: April 24, 1958

Card 4/4

KITAYGORODSKIY, A. I.; STRUCHKOV, Yu. T.; KHORSYANOVA, Tat'yana L'vovna:
VOL'PIN, M. Ye.; KURSANOV, D. N.

"The Crystal Structures of Tropylium Perchlorate and Iodide"

a report presented at Symposium of the International Union of
Crystallography Leningrad, 21-27 May 1959

KITAYGORODSKIY, ALEKSANDR ISAAKOVICH

"Strains and Conformations of Organic Molecules "

A paper/report presented at Symposium of the International Union of
Crystallography, Leningrad 21-27 May 1959

SO: B, 3,135,471

28 July 1959

PHASE I BOOK EXPLOITATION

SOV/3930

Kitaygorodskiy, Aleksandr Isaakovich

Poryadok i besporyadok v mire atomov (Order and Disorder in the World of Atoms)
3rd ed., enl. Moscow, Fizmatgiz, 1959. 150 p. 18,000 copies printed.

Ed.: A.L. Leshchinskii; Tech. Ed.: A.P. Kolesnikova.

PURPOSE: This book is intended for the general reader with an elementary knowledge of physics.

COVERAGE: The book discusses the three states of matter, solid, liquid and gas, and its transformation by liquefaction, evaporation, etc. These processes are examined from the point of view of order or disorder in atoms. Such an interpretation of atomic structure is thought appropriate as some substances are arrangements of particles that can be described as either "orderly" or "disorderly," others are characterized as both "orderly and disorderly" and in these the two are inseparable. Transformations in metals, plastics, or rubber in such technological processes as hardening or mechanical working also produce changes in the order of the distribution of atoms. Thus, the problem of order and disorder in

Card 1/4

Order and Disorder in the World of Atoms

BOV/3930

atoms is a large part of the study of the structure and properties of substances. The book is written in a popular style and contains 65 diagrams and sketches. No personalities are mentioned. There are no references.

TABLE OF CONTENTS:

Introduction	3
Ch. I. Disorder	5
1. What is a disorderly distribution	5
2. Gaseous state of matter	7
3. Thermal movement in gases	9
Ch. II. Order	15
1. Symmetry in the design of wallpaper	15
2. Crystals	20
3. Unseen lattices	22
4. Crystals - tightly packed spheres	25
5. Crystals - not always tightly packed spheres	33
6. Same atoms, but different crystals	41
7. Remote order	43

Card ~~2~~ 4